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Reciprocal mass tensor : a general form

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Using the results of our earlier treatment of wave packets, we have obtained a general form of reciprocal mass tensor. The elements of this tensor are seen to be dependent on momentum as well as space coordinates of the particle under consideration. The conditions under which our tensor would reduce to the usual space-independent form, are discussed And the impact of the space-dependence of this tensor on the motion of Bloch electrons, is examined

1 Introduction

The notion of wave packets is of great importance in quantum-mechanical studies The concept was at first used to investigate quantum-mechanically the motion of free particles, non-relativistic (Messiah 1961, Schiff 1949) as well as relativistic (Bakke & Wergeland 1971) The wave functions used to construct the wave packets for such purposes, are those characterising appropriately the motion of free particles; thus for the non-relativistic case, they are of the form ·

$$\exp i \left[k\,r - \frac{E(\boldsymbol{k})}{\hbar}\,t \right]$$

Later, it was found that the idea of wave packets can, as well, be profitably exploited to study the systems under the action of some internal force. (The Bloch electrons in crystal provide an example) The constituent members of the wave packets relevant to such systems, can no longer be taken as the above-mentioned plane waves; it is, required, instead, to construct these wave packets with such wave functions as actually incorporate the effect of the internal force. Taking this fact into account, we reported, in an earlier communication, a treatment of wavepackets and the formula for the relevant group velocity. Now, we are often required to study systems which are subjected to the action of a uniform external force, besides being acted on by the afore-mentioned internal force. And it is well known that the ideas of reciprocal mass tensor greatly facilitates the investigation of such problems.

In the present article, we have derived the general form of the reciprocal mass tensor for a system which is under the action of an internal force and subjected simultaneously to a uniform external force. The starting point for the work is the formula for the group velocity derived earlier by the author (Roy 1976) This formula for the group velocity and the associated wave packets are summarised in the next section while the section following that one, deals with the derivation of the reciprocal mass tensor. The mass tensor derived here is seen to be dependent on the momentum as well as the space co-ordinates of the system under consideration. The conditions under which the present tensor would reduce to the usual space-independent form are discussed in the last section; there, we also examine the impact of our tensor on the motion of Bloch electrons which serve as a practical example of the type of systems conformable to our treatment

2 Resume of the Wave Packets and the Associated Group Velocity

In this section, we briefly indicate the form of the wave-packet appropriate to the systems of our concern and record also the formula for the relevant group velocity; the details regarding these aspects were reported earlier (Roy 1976)

The wave packets '$\psi(r, t)$' are of the form :

$$\psi(r, t) = \int A(\boldsymbol{k})\phi_{\boldsymbol{k}}(r, t)d^3k \tag{1}$$

where,

$$\phi_{\boldsymbol{k}}(r, t) = u(\boldsymbol{k}, r) \exp i \left[k\, r - \frac{E(\boldsymbol{k})}{\hbar} t \right] \tag{2}$$

$E(\boldsymbol{k})$ is the energy and $u(k, r)$ is an amplitude term dependent on 'k' (with components k_1, k_2 and k_3) as well as the space coordinate 'r' of the system.

The reason we take $\phi(k, r)$ to be what is given by (2), is the fact that this is formally the same as the so-called Bloch waves which govern the motion of electrons in crystalline solids, the latter being subjected to the additional condition . $u(k, r) = u(k, r+R_j)$, where R_j's are lattice vectors Thus, taking $\phi(k, r)$ in the form (2) yields us as easy opportunity of applying our results to the case of Bloch electrons, the treatment of which is one of our objectives. However, in arriving at the results of this as well as the next section, we have not made any use of the above-mentioned Bloch condition on $u(k, r)$. Hence, besides being applicable to Bloch electrons, these results would be valid for any system, the Schrodinger equation of which has solutions in the form or eq (2) The point has been further elaborated later (Discussion).

The group velocity of the wave packets given by eq. (1), was derived earlier by the author (Roy, 1976) The components (V_1, V_2, V_3) of this group velocity (V) are recorded here via the matrix equation (3) below. These forms can be easily obtained from the relations (16), (17) and (18), in the reference just cited

$$\begin{pmatrix} V_1 \\ V_2 \\ V_3 \end{pmatrix} = S \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix} \qquad \dots \tag{3}$$

S is a 3×3 matrix, the elements of which appear as follows

$$S_{11} = \frac{1}{1+\alpha_{x1}}\left[1-\frac{1}{(\gamma_2\delta_1-\delta_2\gamma_1)}\{\alpha_{y1}\alpha_{x2}\gamma_2-\right.$$

$$\left.-\alpha_{z1}\gamma_1\alpha_{x2}+\delta_1\alpha_{x3}\alpha_{z1}\}\right] \qquad \ldots \quad (4)$$

$$S_{12} = \frac{1}{(\gamma_1\delta_2-\gamma_2\delta_1)}[\alpha_{y1}\gamma_2-\alpha_{z1}\gamma_1] \qquad \ldots \quad (5)$$

$$S_{13} = \frac{1}{(\gamma_1\delta_2-\gamma_2\delta_1)}[\alpha_{y1}\delta_2-\alpha_{z1}\delta_1] \qquad \ldots \quad (6)$$

$$S_{21} = \frac{(\gamma_2\alpha_{x2}-\delta_2\alpha_{x3})}{(\gamma_2\delta_1-\gamma_1\delta_2)} \qquad \ldots \quad (7)$$

$$S_{22} = \frac{\gamma_2(1+\alpha_{x1})}{(\gamma_1\delta_2-\gamma_2\delta_1)} \qquad \ldots \quad (8)$$

$$S_{23} = \frac{\delta_2(1+\alpha_{x3})}{(\gamma_2\delta_1-\gamma_1\delta_2)} \qquad \ldots \quad (9)$$

$$S_{31} = \frac{(\gamma_1\alpha_{x2}-\delta_1\alpha_{x3})}{(\gamma_1\delta_2-\delta_1\gamma_2)} \qquad \ldots \quad (10)$$

$$S_{32} = \frac{\gamma_1(1+\alpha_{x1})}{(\delta_1\gamma_2-\gamma_1\delta_2)} \qquad \ldots \quad (11)$$

$$S_{33} = \frac{\delta_1(1+\alpha_{x1})}{(\gamma_1\delta_2-\delta_1\gamma_2)} \qquad \ldots \quad (12)$$

The meanings of the various symbols are given below

$$C_i = \frac{1}{\hbar}\left(\frac{\partial E}{\partial k_i}\right), \qquad i = 1, 2, 3; \qquad \ldots \quad (13)$$

$$\beta_1 = C_1\alpha_{x2}-(1+\alpha_{x1})C_2 \qquad \ldots \quad (14)$$

$$\beta_2 = C_1\alpha_{x3}-(1+\alpha_{x1})C_3 \qquad \ldots \quad (15)$$

$$\gamma_1 = \alpha_{y1}\alpha_{x3}-(1+\alpha_{x1})\alpha_{y3} \qquad \ldots \quad (16)$$

$$\gamma_2 = \alpha_{z1}\alpha_{x3}-(1+\alpha_{x1})(1+\alpha_{z3}) \qquad \ldots \quad (17)$$

$$\delta_1 = \alpha_{x2}\alpha_{y1}-(1+\alpha_{x1})(1+\alpha_{y2}) \qquad \ldots \quad (18)$$

$$\delta_2 = \alpha_{x3}(1+\alpha_{z3})-(1+\alpha_{x1})(1+\alpha_{z3}) \qquad \ldots \quad (19)$$

$$\alpha_{qj} = \frac{\partial}{\partial q}\left(\frac{\partial\alpha}{\partial k_j}\right); \quad q = x, y, z;\ j = 1, 2, 3; \qquad \ldots \quad (20)$$

$$\alpha(\boldsymbol{k}, r) = \text{phase angle of } u(\boldsymbol{k}, r) \qquad \ldots \quad (21)$$

$$= u_1(\boldsymbol{k}, r)+iu_2(\boldsymbol{k}, r). \qquad \ldots \quad (22)$$

3. Presence of Uniform External Force and the Form of Reciprocal Mass Tensor

We want to study now the effect of a uniform external force (F) on a system moving in accordance with the group velocity given by eq (3) When an external force is present, the quantum number 'k' as well as the total energy $E(\boldsymbol{k})$ of the system, change with time. This, in turn, makes the group velocity of the system change with time. Our purpose is to find the rate of change of the group velocity with time and obtain thereby the acceleration of the system under the action of the uniform external force.

To begin with, we derive the rate of change of $\boldsymbol{k}$ with time We have

$$\frac{dE}{dt} = \nabla_k(E)\, \frac{d\boldsymbol{k}}{dt} \qquad \ldots \quad (23)$$

Also,

$$\frac{dE}{dt} = F.V = \sum_{i=1}^{3} F_i V_i \qquad \ldots \quad (24)$$

where, F_i's are the components of F. Restoring in eq (24) the values of V_i's from eq. (3), we have

$$\frac{dE}{dt} = \sum_i T_i \frac{\partial E}{\partial k_i} \qquad (25)$$

where,

$$T_i = \frac{1}{\hbar}\left[\sum_{j=1}^{3} F_j S_{ji} \right] \qquad (26)$$

With the help of eqs. (23) and (25), we get dk_i/dt given as

$$\frac{dk_i}{dt} = T_i; \qquad i = 1, 2, 3; \qquad (27)$$

Taking recourse to eq (3), the i-th component of acceleration (a_i) can be obtained

$$a_i = \frac{dv_i}{dt} = [\, \sum_{j=1}^{3} (C_j \nabla_k S_{ij} + S_{ij} \nabla_k C_j)].\ \frac{d\boldsymbol{k}}{dt}\,. \qquad \ldots \quad (28)$$

Combining eqs. (27) and (28), we finally get

$$a_i = \sum_{n=1}^{3} \left[\frac{1}{\hbar} \sum_{l=1}^{3} \sum_{j=1}^{3} \left\{ C_j \frac{\partial S_{ij}}{\partial k_l} + S_{ij} \frac{\partial C_j}{\partial k_l} \right\} S_{nl} \right] F_n. \qquad \ldots \quad (29)$$

The classical equation of a particle under the action of a uniform force F is given by

$$\frac{d\boldsymbol{V}}{dt} = \frac{\boldsymbol{F}}{m} \qquad \dots (30)$$

We can cast eq (29) in a form analogous to eq. (29), by writing the former as

$$\boldsymbol{a} = \frac{d\boldsymbol{V}}{dt} = \left(\frac{1}{m^*}\right) \boldsymbol{F}. \qquad \dots (31)$$

In eq. (31), $\left(\frac{1}{m^*}\right)$ is the reciprocal effective mass tensor of rank 2. The nine components of this tensor have the following forms .

$$\left(\frac{1}{m^*}\right)_{pq} = \frac{1}{\hbar} \sum_{l=1}^{3} \sum_{j=1}^{3} \left[\left\{ C_j \frac{\partial S_{pj}}{\partial k_l} + S_{pj} \frac{\partial C_j}{\partial k_l} \right\} S_{ql} \right]. \qquad \dots (32)$$

Further, the rule of multiplication of the tensor $\left(\frac{1}{m^*}\right)$ is what is contained in eq. (29).

4 Discussion

Like the group velocity, the form of reciprocal mass tensor derived here is seen to be dependent on the quantum number k as well as the space co-ordinates of the system. The reciprocal mass tensor for free (or quasi-free) particles with energy momentum relation $E(\boldsymbol{k})$, in space-independent and appears as

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j} \qquad \dots (33)$$

The space-dependence of the present tensor is an entirely new feature and owes its origin to the space-dependent amplitude function $u(k, r)$ It is easily noticeable that when u is space-independent, α_{qj}'s are zero and the tensor elemenrs eq. (32) reduce to eq. (33).

The relation (32) expresses in a general way the space-variation of reciprocal mass tensor. Any particular aspect of this space-variation would depend on the explicit form of the amplitude function $u(\boldsymbol{k}, r)$ To elucidate the point, we consider the case of Bloch electrons in crystals. For Bloch electrons, the time-independent part $[u(\boldsymbol{k}, r) \exp(ik.r)]$ of $\phi_k(r, t)$, is the well known Bloch function; the amplitude function $u(\boldsymbol{k}, r)$ satisfies the condition

$$u(\boldsymbol{k}, r) = u(\boldsymbol{k}, r+R_j) \qquad \dots (34)$$

where, R_j's are the lattice vectors. Because of this property of $u(\boldsymbol{k}, r)$, the elements of reciprocal mass tensor are now periodic with periodicities equal to the lattice vectors. It, however appears that the evaluation of electronic properties of crystalline solids on the basis of our mass tensor, would need an averaging with respect to the space coordinates of the electron. The results of the treatment of electronic properties of crystalline solids on the basis of the space-independent mass tensor (33) (Raimes, 1961) would be valid when the amplitude function $u(k, r)$, is slowly varying with r and would come as special cases of those on the basis of the present tensor with. $\alpha_{qj} = 0$

As mentioned above and also earlier, the formulae (3) and (32), for respectively the group velocity and reciprocal mass tensor, are valid for any system, the Schrodinger equation of which has solutions in the form of eq (2). A specific case, where one obtains such solutions, is that of Bloch electrons, the specialities of which have been discussed above It is worth investigating as to what other potentials exist, for which the solutions to relevant Schrodinger equations occur in form of eq. (2) An investigation of this sort would let us know the various kinds of fields which permit the propagation of undispersed wave packets.

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